



Gasoline Combustion Fundamentals

Presenter: Isaac Ekoto
Sandia National Laboratories

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Program Managers: Michael R. Weismiller & Gurpreet Singh
U.S. DOE Office of Vehicle Technologies

Project ID: ACS006

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Overview

Timeline

- Project provides fundamental research supporting DOE/industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VT
- FY18 funding: \$920K
- FY17 funding: \$720K

Barriers identified in VT Multi-Year Program Plan

- Insufficient knowledge base for advanced LTC or mixed-mode combustion systems over the full load range
- Models are needed for fundamental engine combustion and in-cylinder emissions formation processes
- Lack of effective engine control for advanced lean-burn direct injection gasoline engine technology

Partners

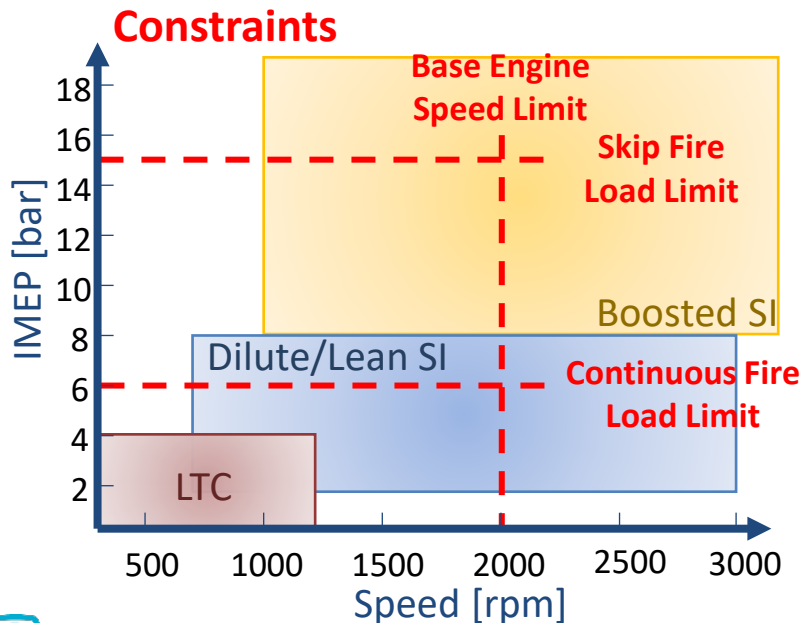
- Project lead: Isaac Ekoto, Sandia National Laboratories
- Industry/Small Business Partners:
 - GM, Ford, John Deere: technical guidance
 - Transient Plasma Systems Inc.
 - 15 Industry partners in DOE Working Group
- University/National Lab Collaborators:
 - Argonne National Lab: Low-temperature plasma modeling
 - U. Orléans (France): Effects of ozone addition on LTC



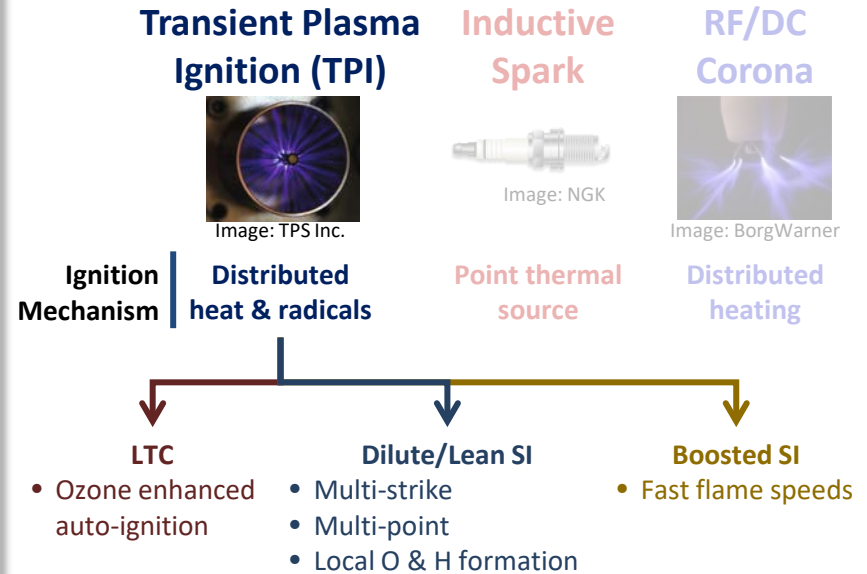
Relevance

Advanced ignition can be a key enabler for clean and efficient next-generation engine combustion.

However, lacking foundational understanding of igniter mechanisms inhibits the development of production-ready systems.



Multiyear Focus: 2016 - present



Turbulent Jet Ignition (TJI)



- LTC**
 - Heat/radical enhanced auto-ignition
- Dilute/Lean SI**
 - Volumetric
 - High-energy
 - Long ignition duration
- Boosted SI**
 - Local flame turbulence
 - Distributed ignition

Objectives

- **Demonstrate** improved low-load engine emissions/efficiency with ozone enhanced LTC, and **identify** the mechanisms that lead to increased fuel reactivity via optical measurements & kinetic modeling
- **Quantify** transient plasma discharge products and ignition behavior at relevant conditions, with the data used to **validate** complementary discharge simulations (ANL – ACS075)
- **Fabricate** new transient plasma & turbulent jet igniters developed from a rigorous design review process, along with instrumented test facilities that feature well-controlled boundary conditions and optical access for *in situ* measurements

Impact: Project reveals fundamental mechanisms of advanced ignition systems for next-generation gasoline engines, which enables more informed implementation and faster commercialization.



Approach & Milestones

1. Identify promising igniter technology

- Transient Plasma Ignition (TPI): **FY15 – present**
- Turbulent Jet Ignition (TJI): **FY17 – present**

2. Develop hardware & diagnostics

- Optical calorimeter: **FY16**
- O-atom TALIF @ pressure: **FY17-18**
- TPI plug: **FY16 – present**
- Ozone absorption: **FY17-FY18**
- Optical ignition chamber: **FY18Q3**
- TJI Engine Head: **FY17Q4**
- TJI plug: **FY18Q4**

3. Fundamental experiments

- Calorimetry: **FY16 – present**
- Optical emission: **FY16 – present**
- TPI O-atom TALIF: **FY18Q1**
- TPI Ignition sampling: **FY18Q3**
- Flame development: **FY18Q4**
- RCM ozone absorption: **FY18Q1**

4. Model observed behavior

- Ozone kinetic modeling: **FY18**
- ANL TPI simulations: **FY17 - present**

5. Engine Tests: Performance

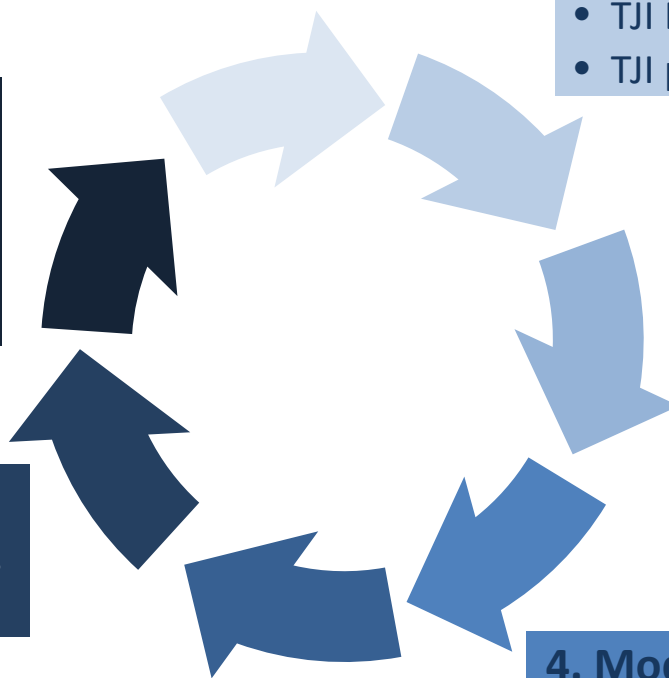
- LTC w/ ozone-addition: **FY17 – present**
- Retarded ST TPI: **FY18**

6. Engine Tests: Optical

- Ozone absorption: **FY18Q1**
- TPI imaging: **FY18Q3**

7. Review

- TPI electrode down-select: **FY18Q2**
- TJI conceptual model: **FY19**



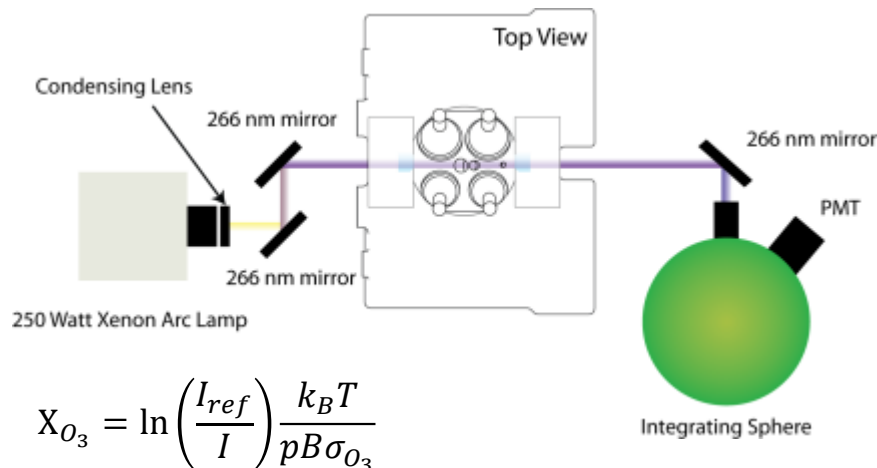
Accomplishment: Diagnostic & hardware development

1. Ozone Absorption: Enables crank angle resolved bulk in-cylinder ozone concentration measurements

2. O-atom (TALIF): First quantitative measure of TPI generated O-atom at engine-relevant conditions

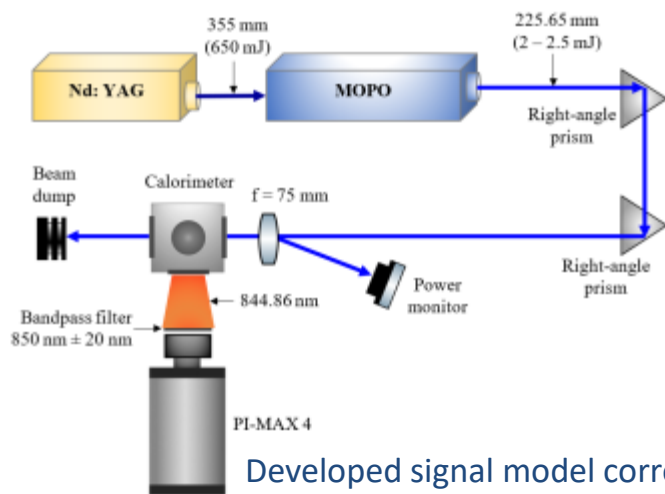
3. Transient Plasma Plug: Redesigned plug eliminates surface discharge issues from previous design

1



2

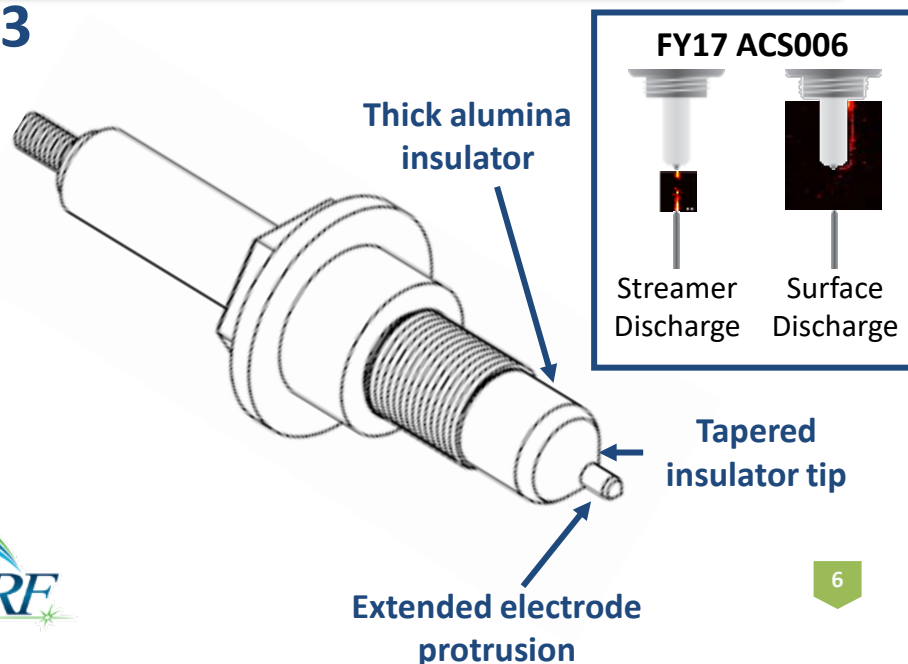
Gordon Research Conference Invited talk – Aug 2017



Developed signal model corrects for **pressure-broadening & stimulated emission**

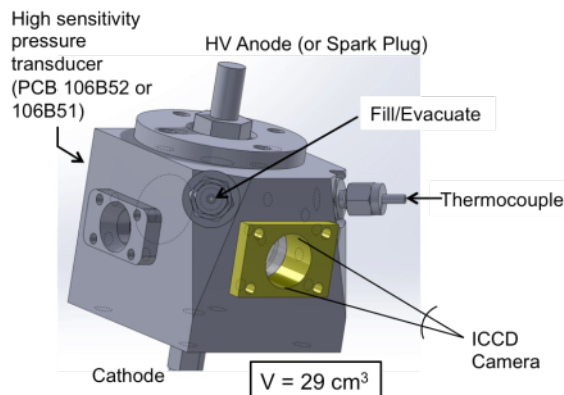


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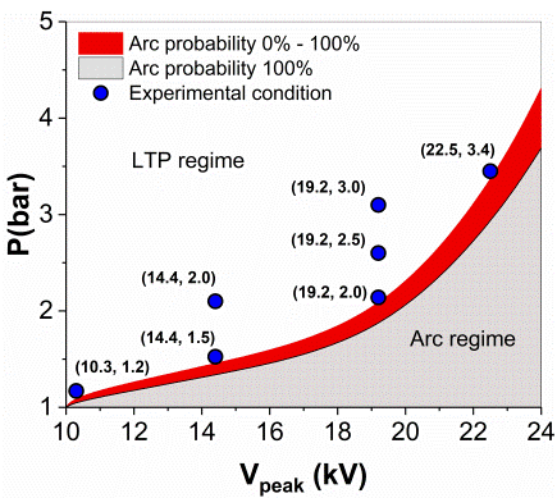


Accomplishment: Quantified transient plasma discharge behavior (1/3)

Optically-Accessible Ignition Calorimeter

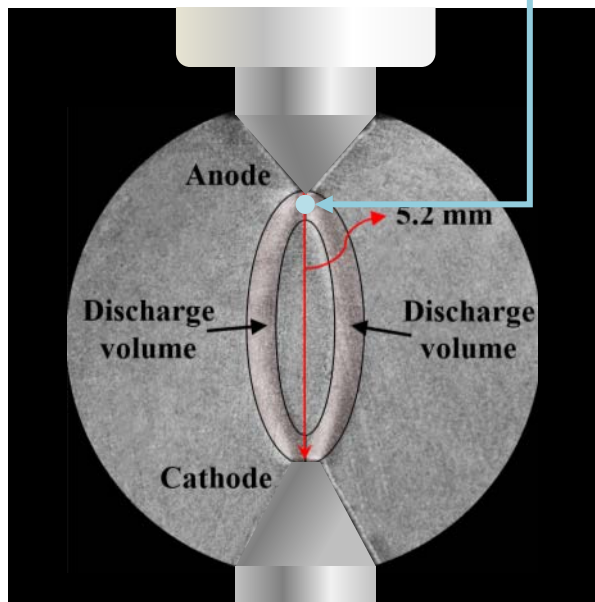


Range of peak discharge voltages & pressures explored



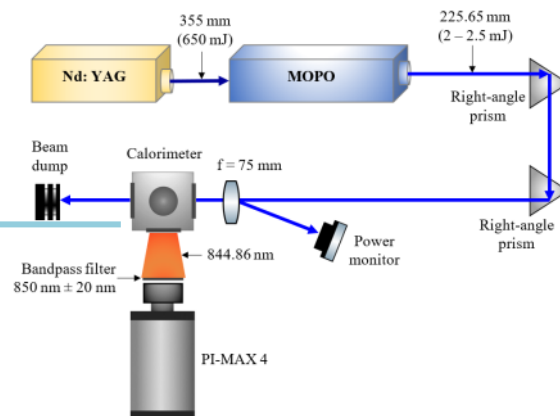
Transient Plasma Characteristics

- Pin-to-pin electrodes
- ~12 ns discharges
- 5 – 20 mJ/pulse



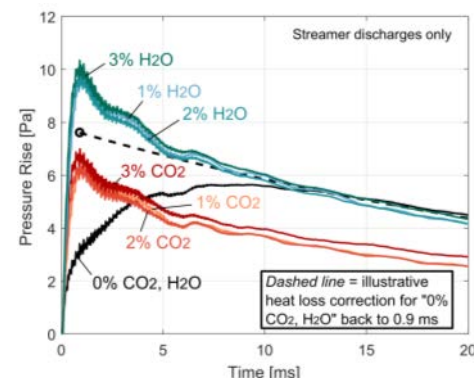
Schlieren imaging

- Discharge volume
- Channel temperature (w/ calorimetry)
- Flame kernel growth



O-atom TALIF

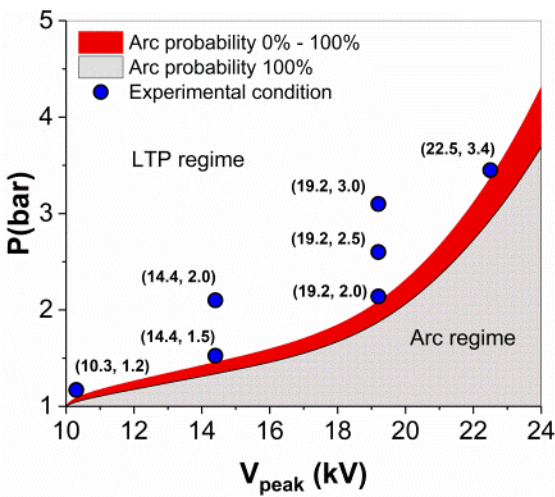
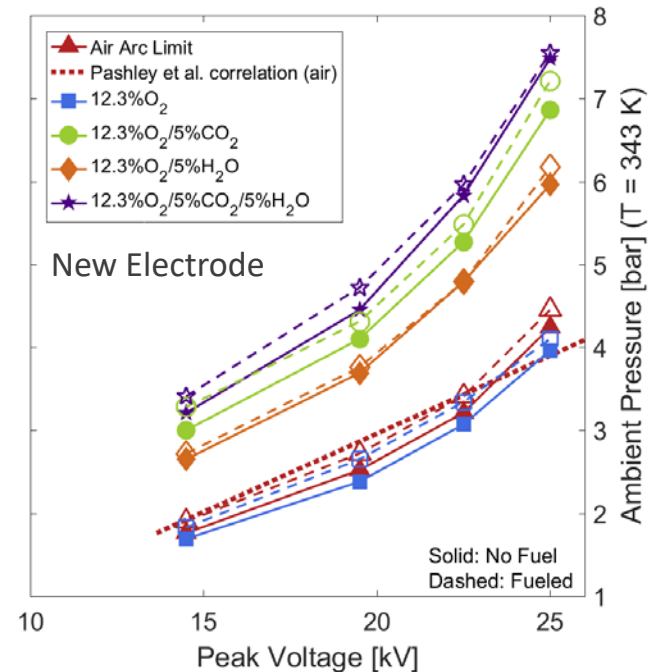
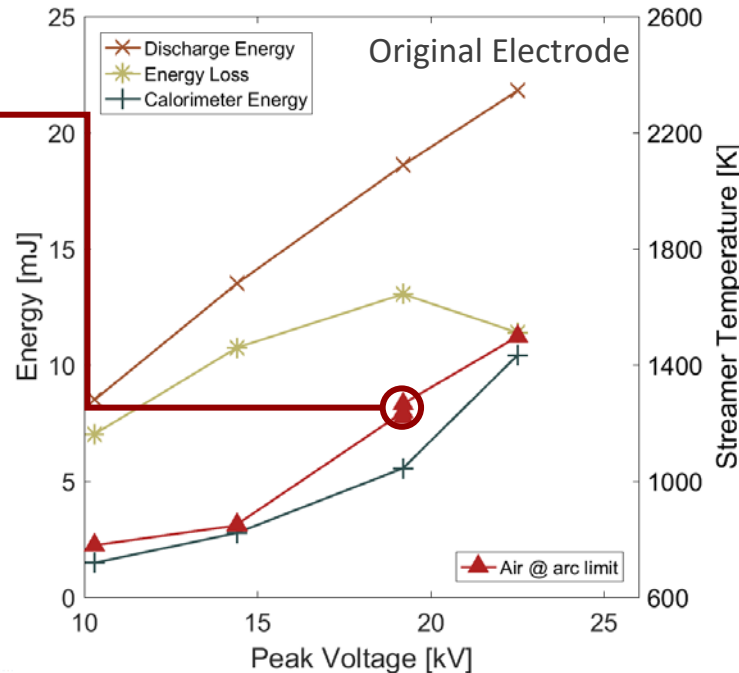
- Quantitative O-atom conc.



Plasma Discharge Calorimetry

- Localized gas heating

Accomplishment: Quantified transient plasma discharge behavior (2/3)



- Non-linear increase in thermal energy deposition with V_{peak}
 - Initial heating occurs in dual streamer filaments
 - Thermal deposition independent of initial pressure/composition
- Breakdown limits match empirical correlations: SAE 2000-01-0245
 - Pulse duration (~12 ns FWHM) not short enough to avoid breakdown
- EGR and fuel addition also match previous observations

Accomplishment: Quantified transient plasma discharge behavior (3/3)

Effect of peak voltage:

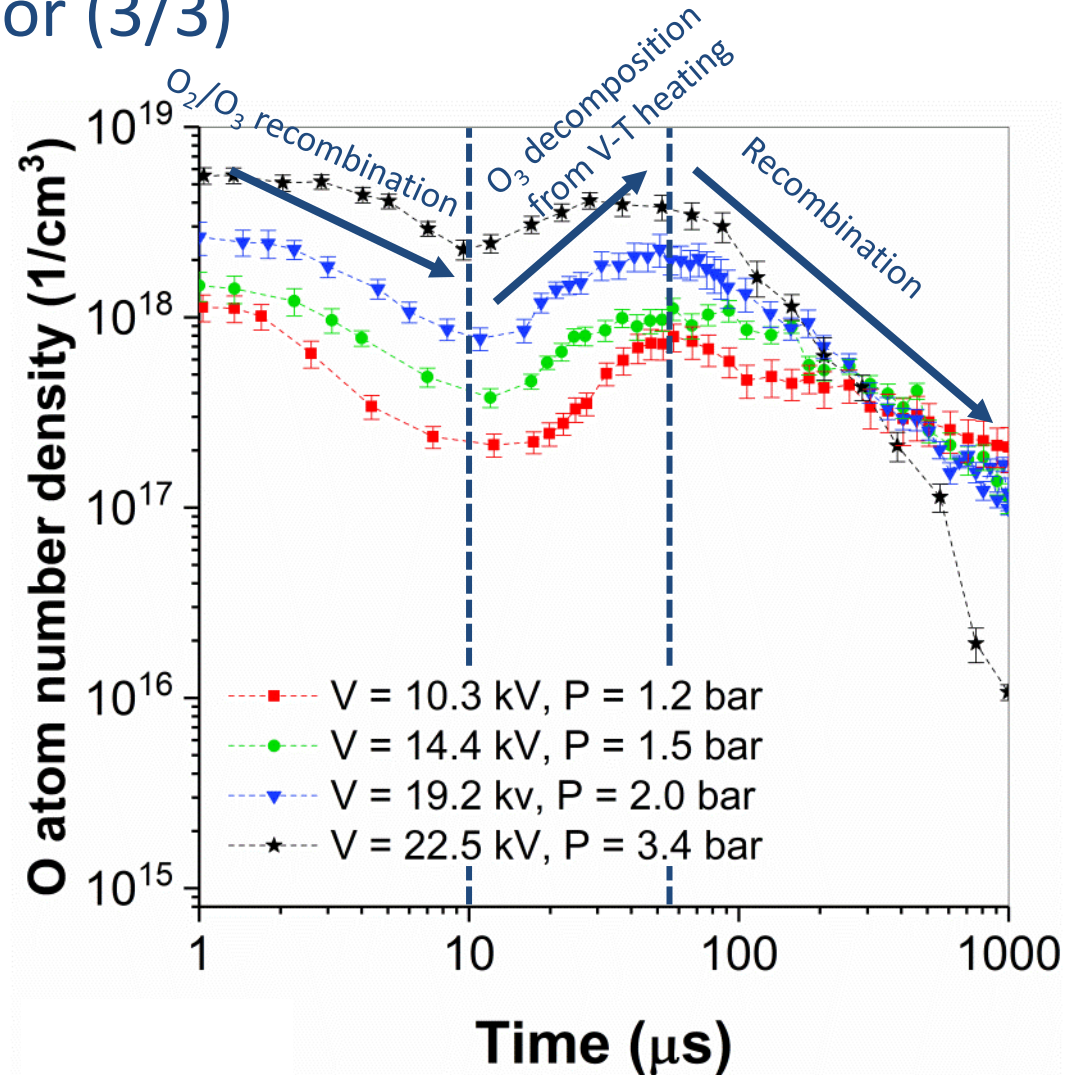
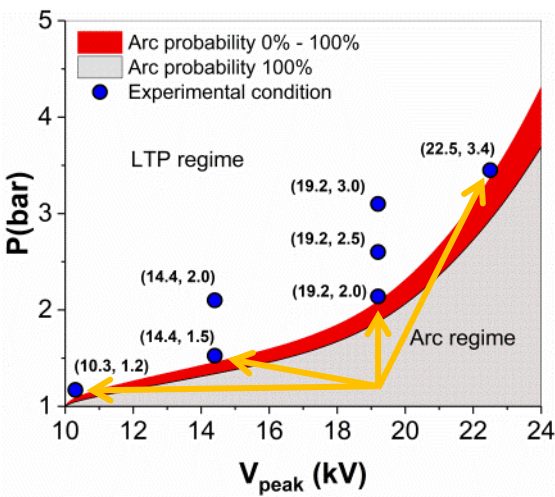
- V_{peak} : $\downarrow 25\% \Rightarrow E_{\text{cal}}$ & O-atom $\downarrow 50\%$

Effect of initial pressure:

- P_{ini} : $\uparrow 25\% \Rightarrow$ O-atom $\downarrow 50\%$
- P_{ini} : $\uparrow 50\% \Rightarrow$ O-atom $\downarrow 75\%$
- Thinner streamers w/ higher pressures

Arc limit:

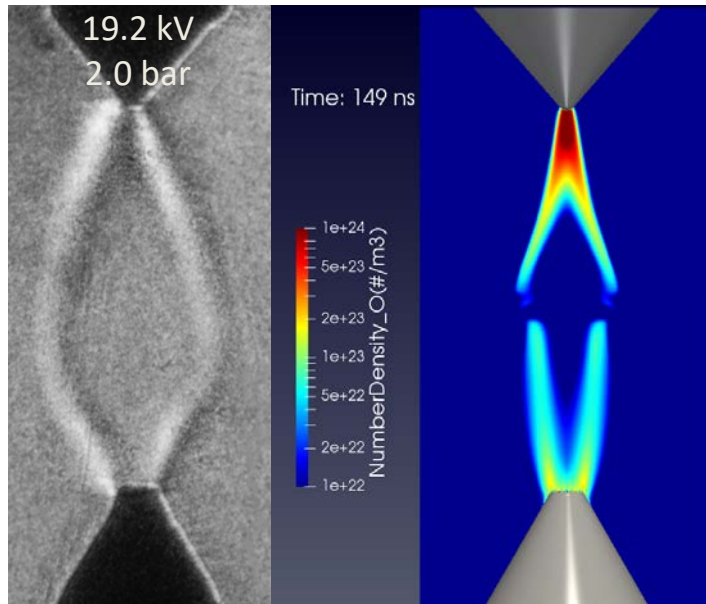
- O-atom concentrations greater than 10%
- Faster recombination w/ $\uparrow P_{\text{ini}}$



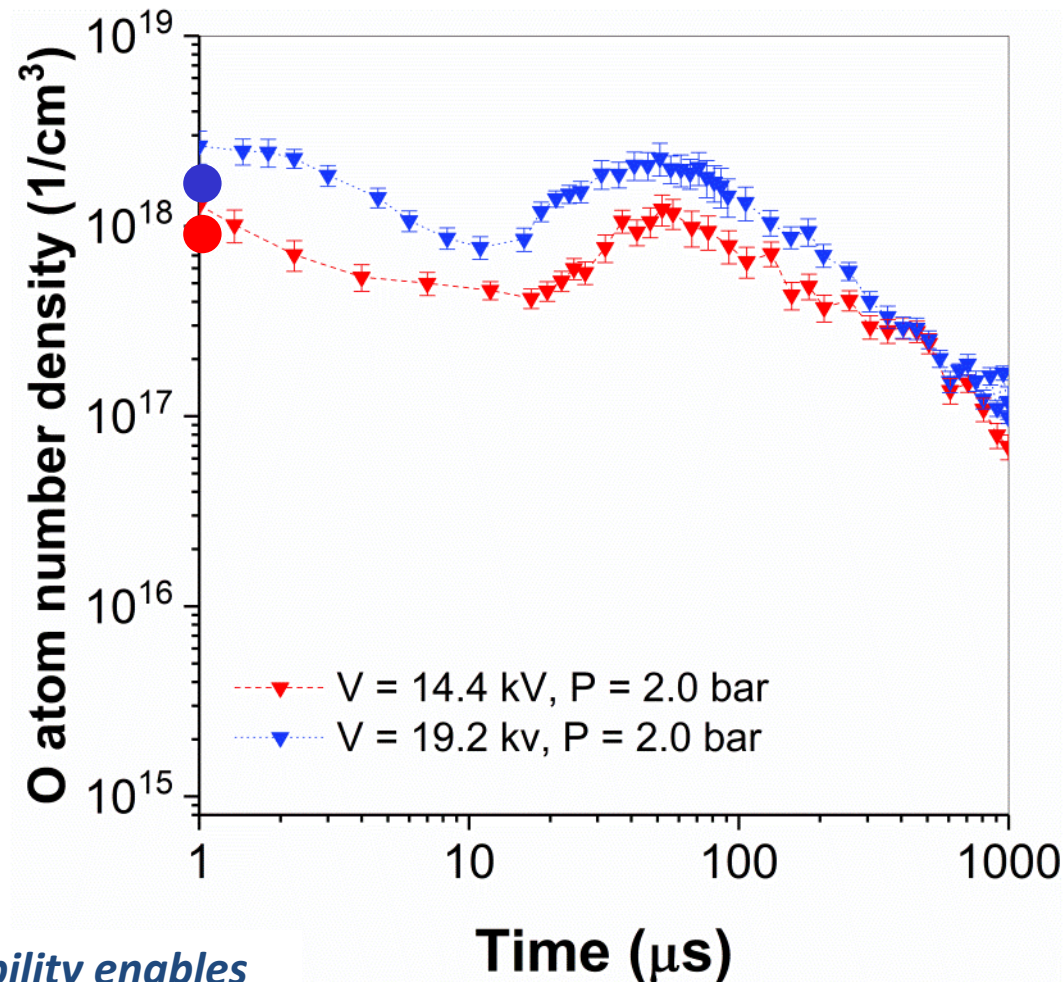
Impact: Transient plasma modeling benchmarks obtained for relevant in-cylinder conditions

Accomplishment: Modeling transient plasma discharges

Modeling data/images from Riccardo Scarcelli (ANL) ACS0075



- Excellent qualitative agreement in streamer structure & behavior
- Quantitative O-atom concentrations are also well-matched
 - Correct trends likewise captured



Impact: *Validated LTP modeling capability enables more rapid optimization of discharge characteristics & electrode configurations.*

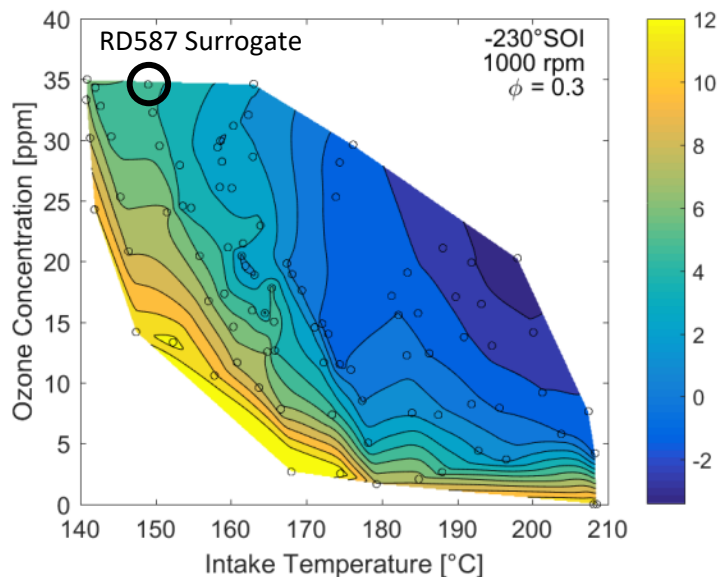
2017 US DRIVE technical accomplishment

Accomplishment: Clarified the mechanisms of O₃ enhanced auto-ignition for gasoline LTC (1/3)

	Sandia Engine
Combustion Mode	Compression Ignition
Engine Design	Spray Guided
Injector	Central VCO
Displacement [L]	0.55
Stroke/Bore	1.11
Compression Ratio	13
Intake Pressure [bar]	1
Intake O ₃ Conc. [ppm]	0 – 40
Equivalence Ratio	0.3
IMEP [bar]	~2.8

Fuels Tested	Iso-Octane	1-Hexene	RD587 Gasoline	†RD587 Gasoline Surrogate
LHV [MJ/kg]	44.4	44.4	41.9	41.9
H/C ratio	2.25	2	1.97	2.01
RON	100	76.5	92.1	~92
Octane Sensitivity	0	13.1	7.3	~7
T10/T50/T90 [°C]	99.3	63.4	57/98/156	91/96/103

†Volume Fraction: 46.6% IO, 17.8% nH, 9.9% EtOH, 6.0% 1-Hex, 19.7% Tol



CA50 insensitive to SOI

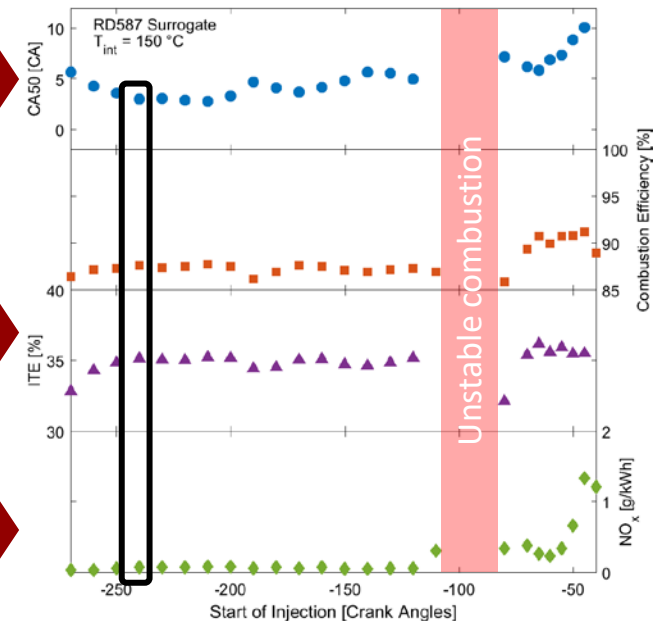
CA50 correlates with ITE & CoV of IMEP

Up to 85° C lower T_{int}

Good low load ITE (~2.8 bar IMEP)

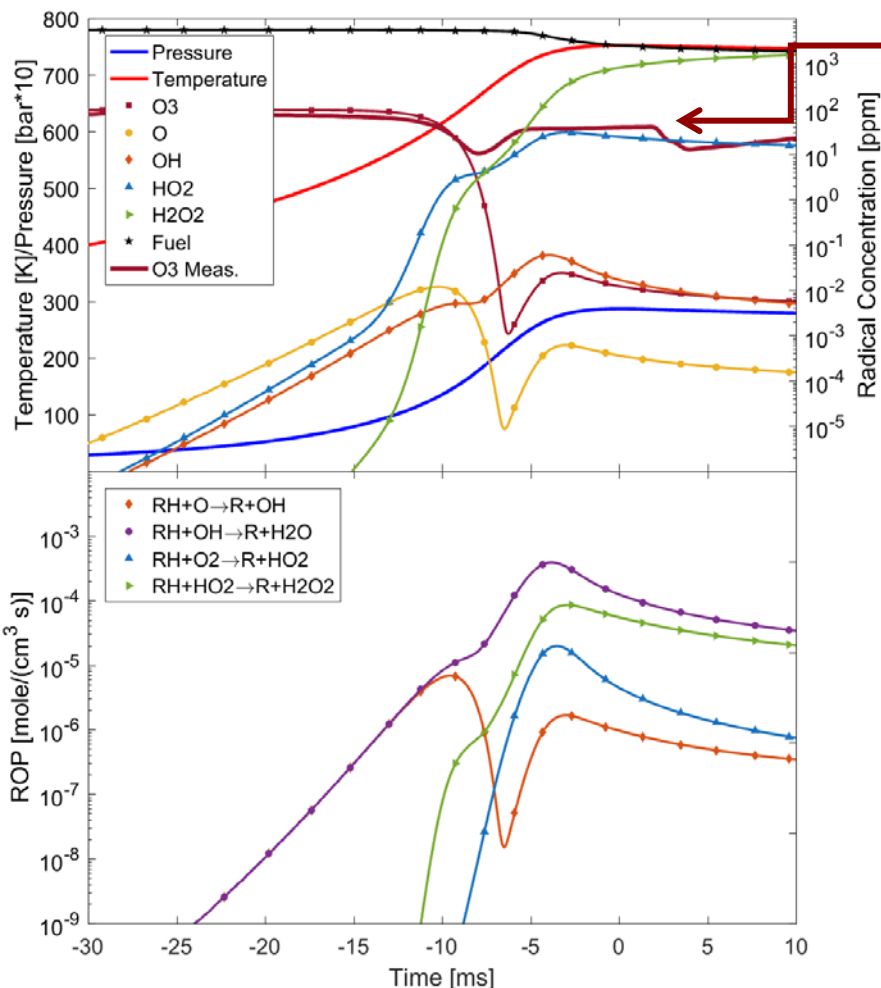
Wide CA50 control authority ($\pm 5^\circ$)

Low NO_x



Similar trends observed with iso-octane & 1-hexene fueling

Accomplishment: Clarified the mechanisms of O₃ enhanced auto-ignition for gasoline LTC (2/3)



Secondary UV absorbance from low- & high-temperature heat release (LTHR/HTHR) intermediates (i.e., HO₂ & H₂O₂)

Masurier et al., *Energy & Fuels*, 27 (9):5495, 2013

Decomposition/Recombination

Fast recombination rxn. ➡

1. $O_3 + O_2 \leftrightarrow O_2 + O + O_2$
2. $O_3 + N_2 \leftrightarrow O_2 + O + N_2$
3. $O_3 + O_3 \leftrightarrow O_2 + O + O_3$

Fuel Oxidation

Accelerated HO₂/H₂O₂ Rate of Production ➡

4. $RH + O \leftrightarrow R + OH$
5. $RH + OH \leftrightarrow R + H_2O$
6. $RH + O_2 \rightarrow R + HO_2$
7. $RH + HO_2 \rightarrow R + H_2O_2$

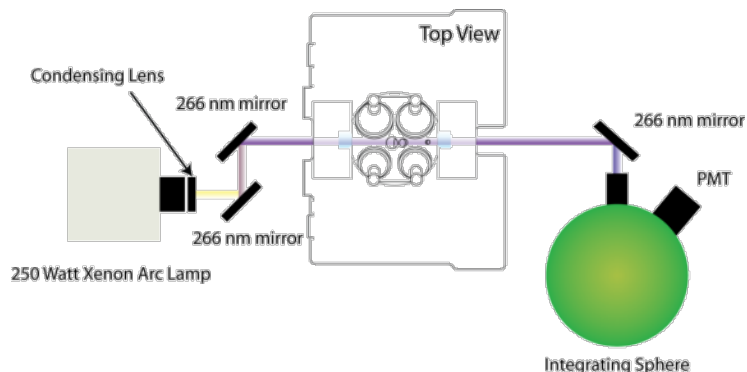
Model captures correct fuel-air mixture reactions, but needs updated rate constants & H₂O/CO₂ decomposition reactions for EGR mixtures



U. Orléans Optically Accessible
Rapid Compression Machine

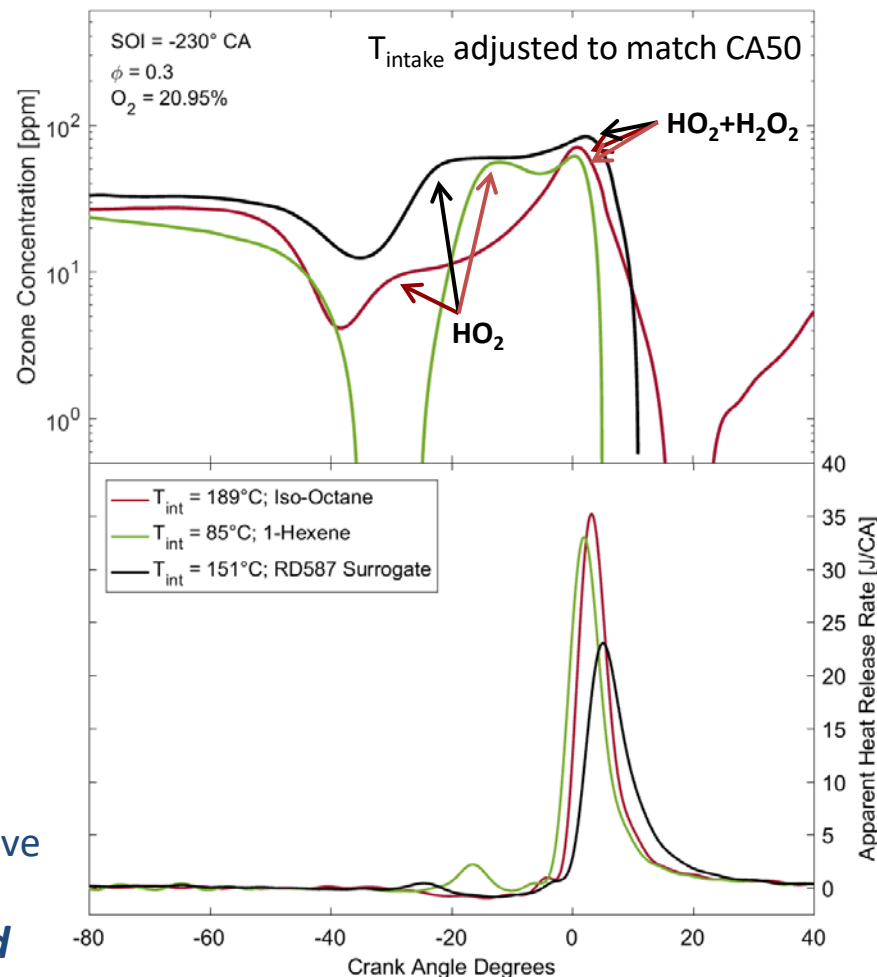


Accomplishment: Clarified the mechanisms of O₃ enhanced auto-ignition for gasoline LTC (3/3)

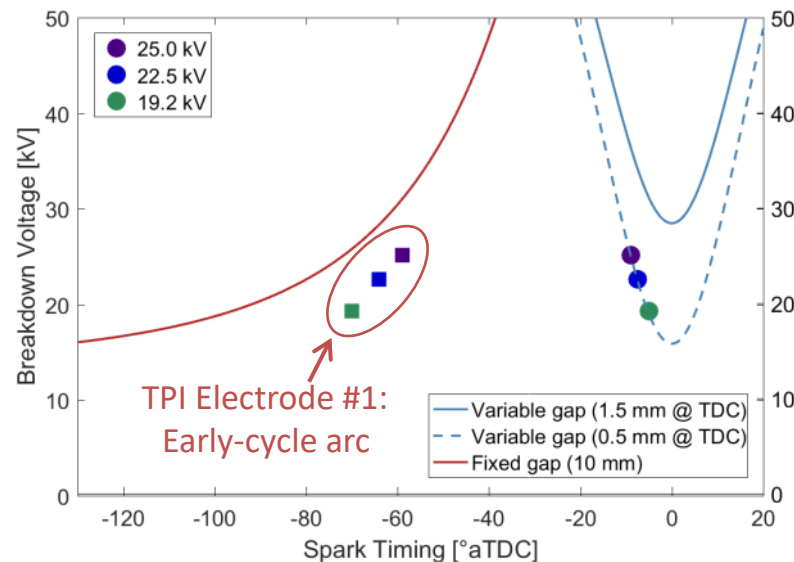
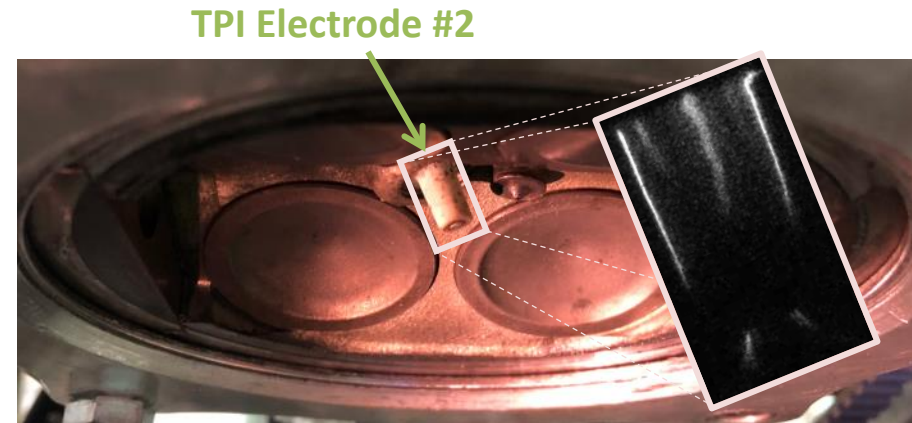
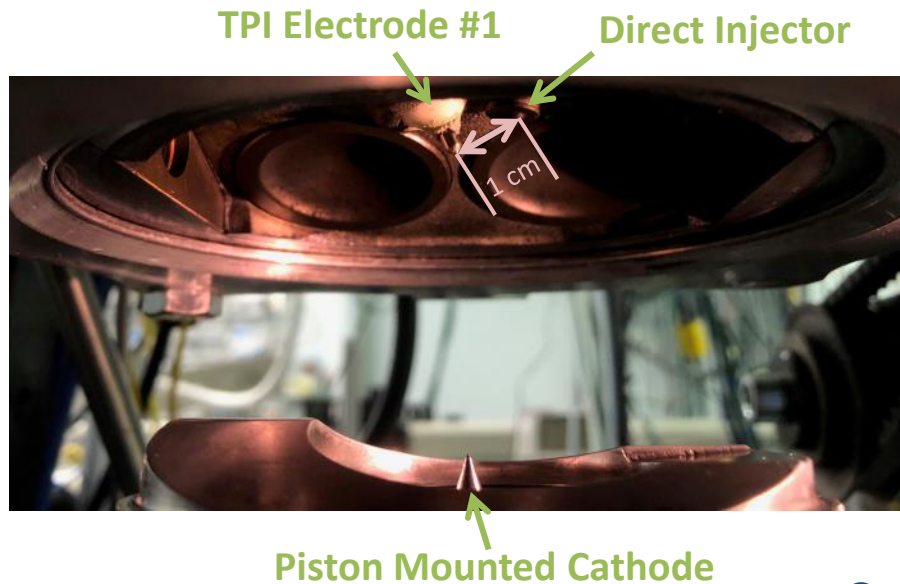


- Fast H abstraction \Rightarrow slow O+O₂ recombination \Rightarrow accelerated O₃ decomposition
 - Process depends on fuel C-H bond types
- UV absorbance correlates w/ LTHR & HTHR rxns.
- O₃ addition accelerates LTHR
 - **1-Hexene**: Strong LTHR despite high OS
 - **RD587 Surrogate**: Moderate LTHR
 - **Iso-octane**: LTHR is too fast & becomes less effective

Impact: Improved understanding of O₃ enhanced auto-ignition enables the development of predictive kinetic models



Accomplishment: Engine Transient Plasma Ignition (1/2)

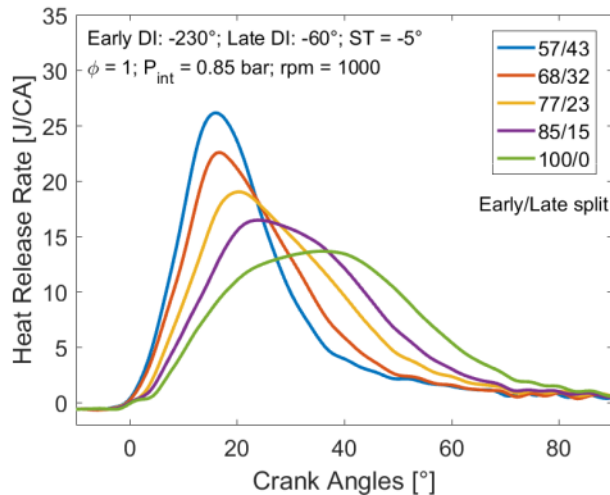


Goal: Early-cycle O_3 formation; late-cycle SI

- Piston mounted cathode to avoid early-cycle arc
- Minimum calculated V_{BD} occurs @ TDC
 - Actual V_{BD} ~10 kV lower → **FY17: pulse reflection arcs**
- **TPI electrode #1:** Early-cycle arc to the injector
- **TPI electrode #2:** Flush tip & thinner insulator
 - Eliminates early-cycle arcs
 - Piston cathode preserved
 - O formation now along insulator surface

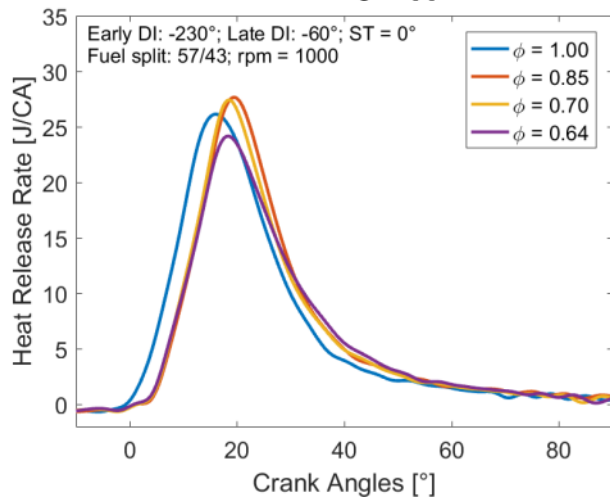
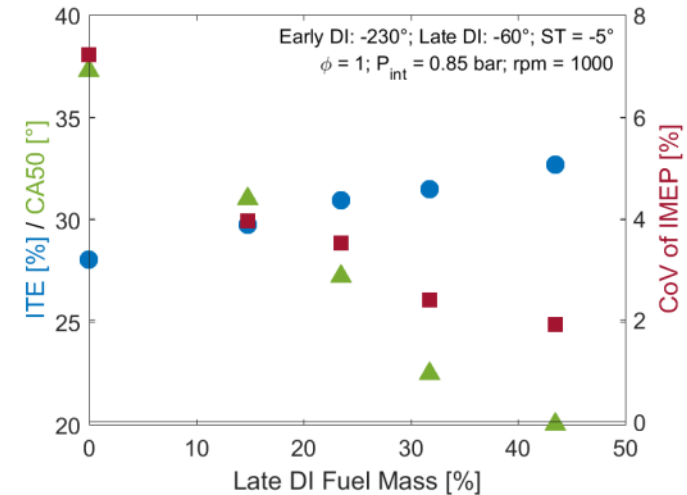
Accomplishment: Engine Transient Plasma Ignition (2/2)

- Breakdown required for ignition; only possible for ST within 5° of TDC



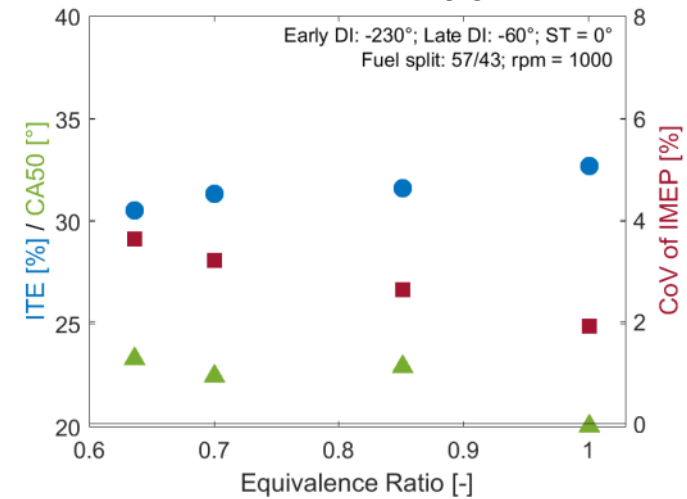
← All DI fuel splits ignited

Poor stability w/ higher early DI factions →



← Robust ignition for all ϕ

Lower lean charge ITE from combustion retard →



Need higher pulse voltages to advance spark timing and achieve true LTP ignition (TPS will provide in FY18Q4)

Reviewer Response

Q1 R4: Perhaps the project should adopt a more pragmatic approach to studying ignition systems.

Response: We appreciate the need for expediency, but our opinion is that previous advanced ignition studies have led to erroneous or sub-optimal findings precisely because the igniter operating principles were poorly understood or the combustion system was poorly adapted to the igniter characteristics. An example is the TPI thermal hysteresis effect we documented in FY17 that leads to arc during multi-pulse operation. In FY18 we explored the effect of TPI in an engine, but always with an eye toward acquiring data useful for creating/validating complementary modeling efforts.

Q2 R3: The team needs to develop plans to quickly identify the go/no-go decision points on this approach.

R4: Is there a way to accelerate the pace of work and results?

Response: The transition from NVO HCCI to ignition system work has taken time due to the requirement to completely retrofit an engine lab to perform relevant advanced ignition measurements. In the ~18 months since the retrofit was completed, we have acquired impactful data and developed new understanding related to the use of advanced plasma igniters, with the results already published. Complementary ignition physics work performed in FY16/17 has accelerated our comprehension of new engine data and has allowed us to quickly down-select igniter configurations as discussed in this presentation.

Q4 R2: Future work should focus on the fundamental measurements of the ignition system to provide detailed information for ignition system sub-models for combustion simulations.

Response: In FY18 we acquired numerous challenging measurements related to plasma-assisted ignition within our optically accessible spark vessel at engine relevant conditions. We likewise explored the kinetics of O₃ addition on auto-ignition chemistry within both our optical engine and with a collaborator's RCM. These data have been widely shared with OEM partners and already used to update ignition/combustion simulation sub-models.

Q5 R3: Quantity of work over the last few years has been minimal and has had minimal impact.

Response: While we respect vast expertise of the reviewers, we strenuously disagree with this characterization of the project. Despite having to rebuild an engine lab, numerous studies have been published in the past 4 years (an average of 4/year) that have been well received by academic and industry researchers alike. Project research has directly led to multiple invited talks, the SAE PFL Best Paper Award (2015), 3 US DRIVE technical highlights (1 in 2016 and 2 in 2017), and the SAE Harry L. Horning Award (2016). Moreover, we have directly engaged with industry researchers and tailored our research directions to be responsive to their needs. This included direct sharing of data/models/results along with our unvarnished opinion of what it all means. In short, while we always aspire to do more, we feel the quality and quantity of our work stands for itself.



Collaborations

- National Lab
 - Argonne National Laboratory (ACS075):
 - Shared validation data in support of advanced ignition modeling
 - Sandia National Laboratories' Applied Optical/Plasma Science Dept. :
 - Shared results and solicited advice on LTP discharge experiments
- University
 - U. Orléans:
 - 3-month sabbatical by Prof. Fabrice Foucher to perform joint experiments into the influence of ozone-addition on LTC
 - Arkansas Tech:
 - DOE EPSCoR proposal submitted to look at light-activated nanoparticle ignition
- Automotive OEM and Suppliers
 - General Motors:
 - Regular technical interactions: 1) results exchange, 2) hardware support, 3) feedback on research directions
 - Joint TJI experiment planning with a common single-cylinder research head (w/ Mich. State)
 - Shared in-cylinder ozone experiment data for model development
 - Ford:
 - Intermittent technical discussion on LTP ignition: 1) results exchange, 2) feedback on research directions
 - John Deere:
 - Kinetics of in-cylinder ozone addition
- Small business
 - Transient Plasma Systems Inc.:
 - Data and hardware sharing
 - Electronics design and maintenance support for high-voltage nanosecond pulse generators
 - DOE Advanced Manufacturing Office proposal submitted to evaluate TPI for large-bore natural gas engines
 - Tula Technologies:
 - Preliminary discussion on hardware modifications needed to enable cylinder deactivation on our single-cylinder research engine
 - Esgee Technologies:
 - Joint publication of 2 papers on multi-physics modeling of nanosecond LTP
- DOE Working Group
 - Shared research results and insights at DOE's Advanced Engine Combustion project review meetings.



Remaining Challenges and Barriers

- **TPI design/operation**: Is arc required for certain TPI conditions?
 - Can shorter (~ 1 ns), close coupled (~ 50 kHz) pulses better avoid arc?
 - Can O_3 facilitate dilute spark-assisted CI for moderate speeds/loads?
 - Is O_3 more effectively generated in streamers or along the electrode insulator?
 - Can igniter generated O_3 be modeled? What are the associated energy requirements?
- **Ozone kinetics**: How does NO , H_2O , and CO_2 impact O_3 addition kinetics?
 - Are there opportunities for post-combustion emissions abatement with O_3 ?
- **Turbulent Jet Ignition**: What is the mechanisms for ignition?
 - What is the interplay of jet-strength, radical generation, and heating on ignition?
 - How sensitive are ignition characteristics to what goes on in the pre-chamber?
- **Advanced Ignition & Dynamic Skip Fire (DSF)**: Can TJI/TPI improve DSF?
 - Can advanced ignition allow for higher firing frequencies at lower load per fire to achieve the same fuel consumption with better NVH?



Future Work

- TPI design/operation :

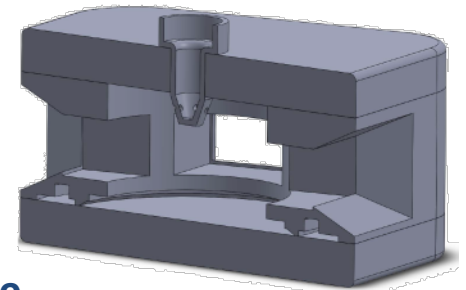
- Evaluate 50 kV_{peak} pulse generator w/ multi-pulse in the engine: **Q4FY18**
- Compare effect of protruded vs. flush anodes & fixed vs. variable gaps: **Q4FY18**

- Ozone kinetics:

- Evaluate the impact of EGR constituents: **FY18 /19**
- Quantify O₃ generation from TPI for various pulse strategies: **Q3-Q4FY18**
- Work w/ modelers to update mechanisms & model discharge generated O₃: **FY18 /19**

- Turbulent Jet Ignition:

- Complete design & construction of TJI ignition test facility (details in Technical Backup Slides): **Q4FY18**
- Visualize chemical/mixing field where ignition occurs: **Q1FY19**
- Evaluate impact of jet strength vs. jet products on ignition: **FY19**
- With GM R&D, procure/develop suitable prototype head mounted TJI systems: **FY19**



- Advanced Ignition w/ DSF:

- Identify valve-train hardware needed for cylinder-deactivation studies in existing optical engine: **FY19**

Summary

Relevance

- Project reveals the fundamental mechanisms of advanced ignition systems for next-generation gasoline engines, which enables more informed implementation and faster commercialization

Approach

- Remove new igniter commercialization barriers through targeted engine and well-controlled vessel experiments, with complementary modeling by lab/university/OEM partners

Technical Accomplishments

- New hardware/diagnostic capabilities developed (O_3 absorption, O-atom TALIF, TPI igniter)
- 35 ppm of added O_3 found to reduce gasoline LTC intake heating requirements by up to 85°C through accelerated LTHR kinetics
- Measured crank-angle resolved O_3 concentrations for different dilution ratios, intake temperatures, and fuels; data used to update kinetic models

- TPI breakdown voltages found to be consistent with developed correlations for conventional spark discharges; i.e., 12 ns FWHM pulses is not truncated enough to avoid breakdown
- First-ever quantitative measure of LTP generated O-atom at engine relevant conditions; results used to improve/validate complementary ANL discharge simulations (ACS075)
- Tested new TPI igniters in the optical engine:
 - Protruded electrode easily arced to engine surfaces
 - Flush electrode better avoids undesirable arc, and may more effectively produce O_3 along the insulator
 - Robust ignition observed with retarded spark timing

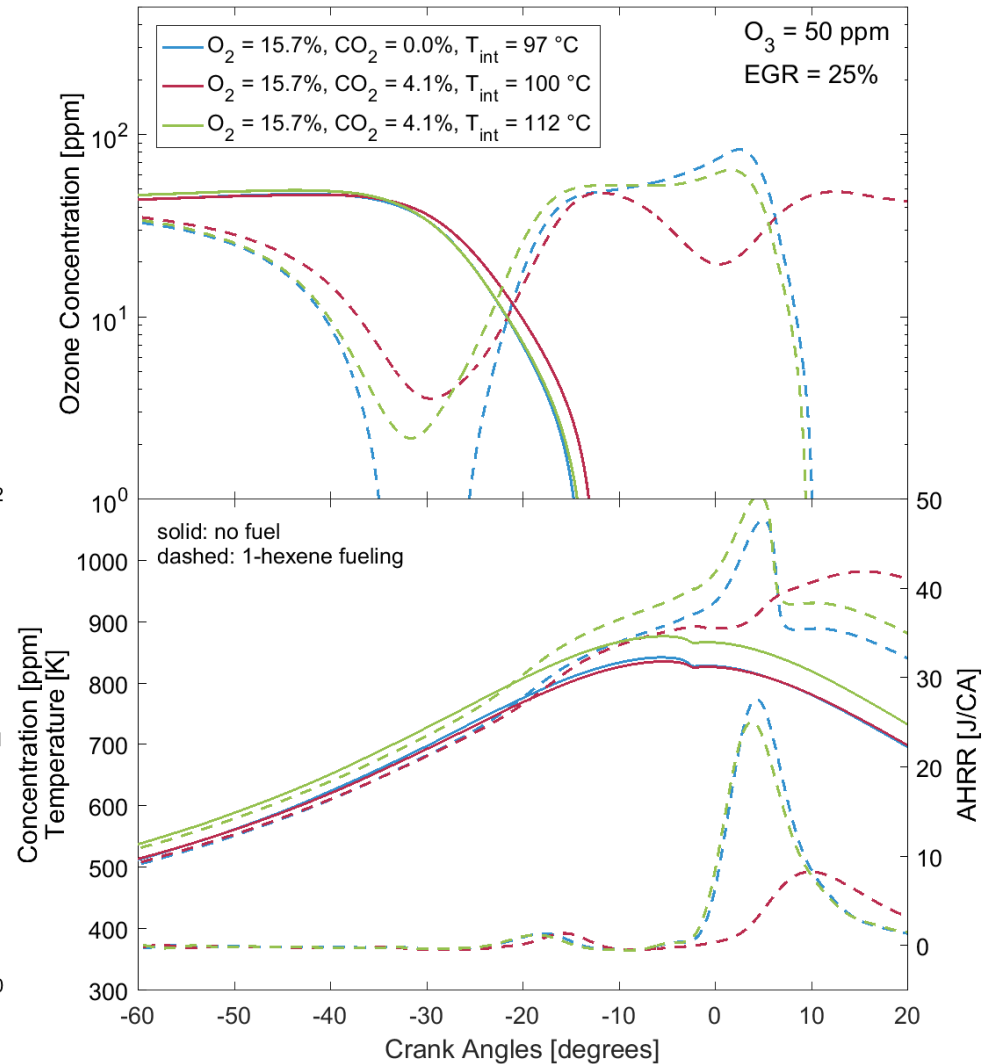
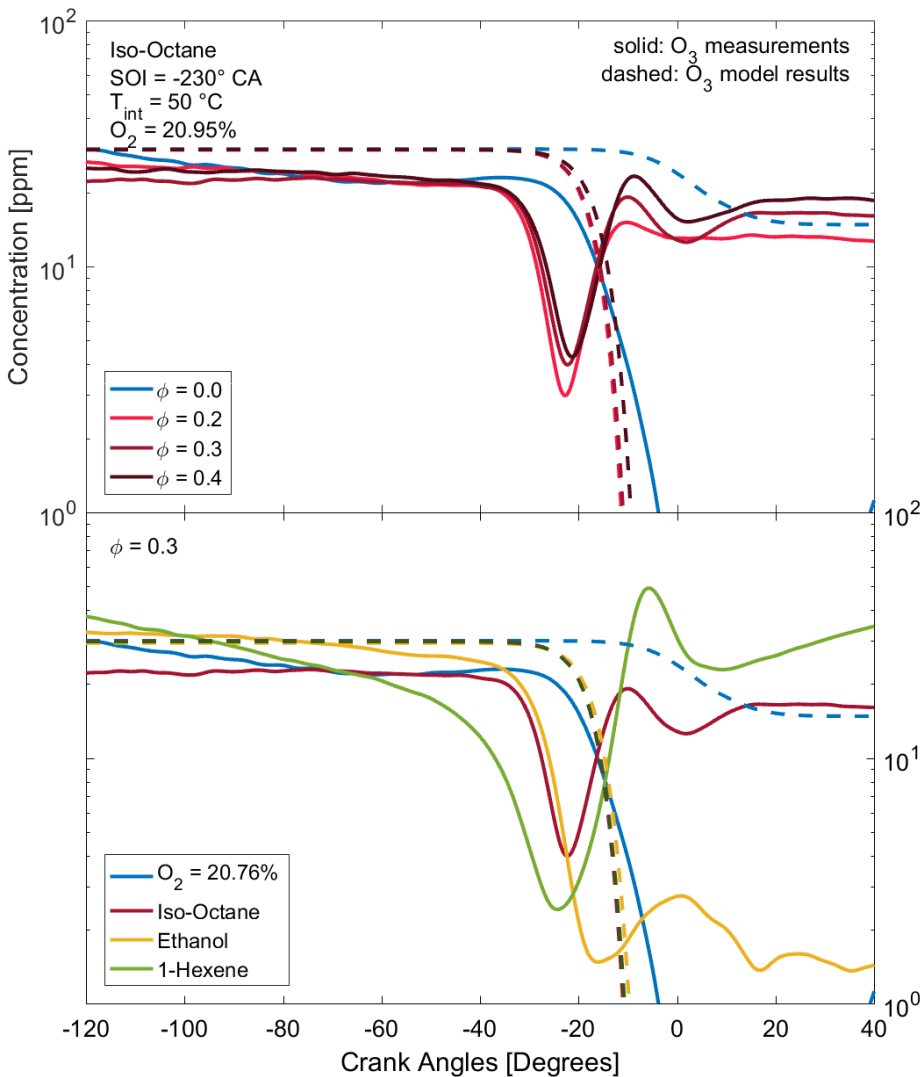
Proposed Future Research

- Work with ANL to model O_3 fuel/EGR interactions
- Identify key TPI parameters for lean/dilute SI
- Evaluate how O_3 addition influences SACI
- Complete construction of TJI test vessel & explore ignition mechanisms for various parameters
- Start cylinder-deactivation valve-train hardware integration



Technical Backup Slides

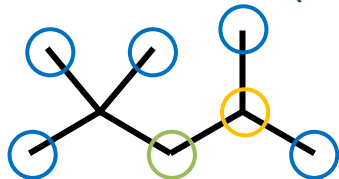
Effects of ϕ , fuel type, and EGR on O_3 decomposition



Estimating H abstraction rates by O for different fuels.

- Vinyl
- Primary
- Secondary
- Tertiary
- Allylic

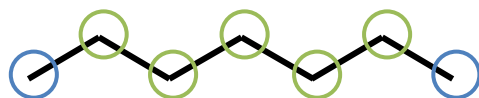
Iso-Octane: 35% (46.6 vol%)



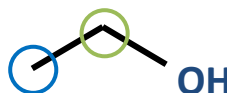
1-Hexene: 6% (6.1 vol%)



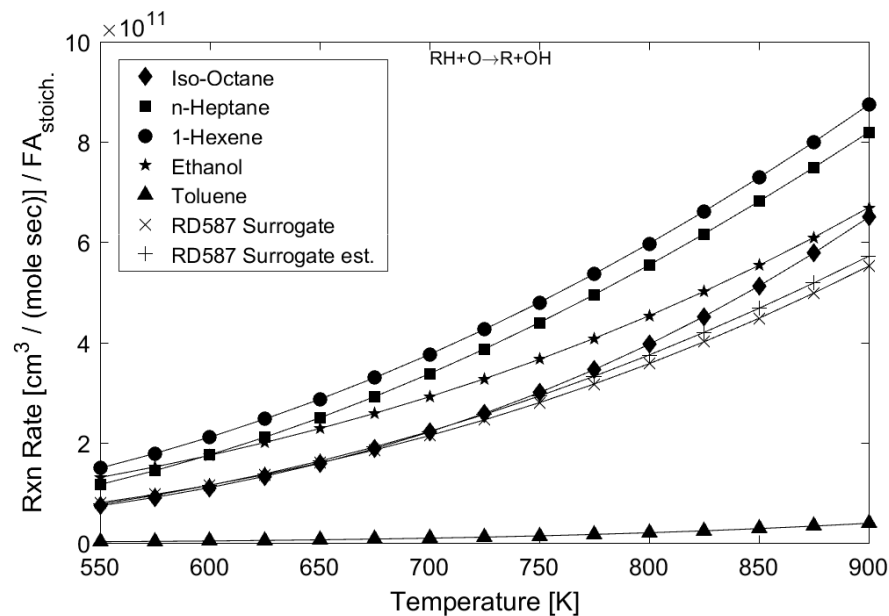
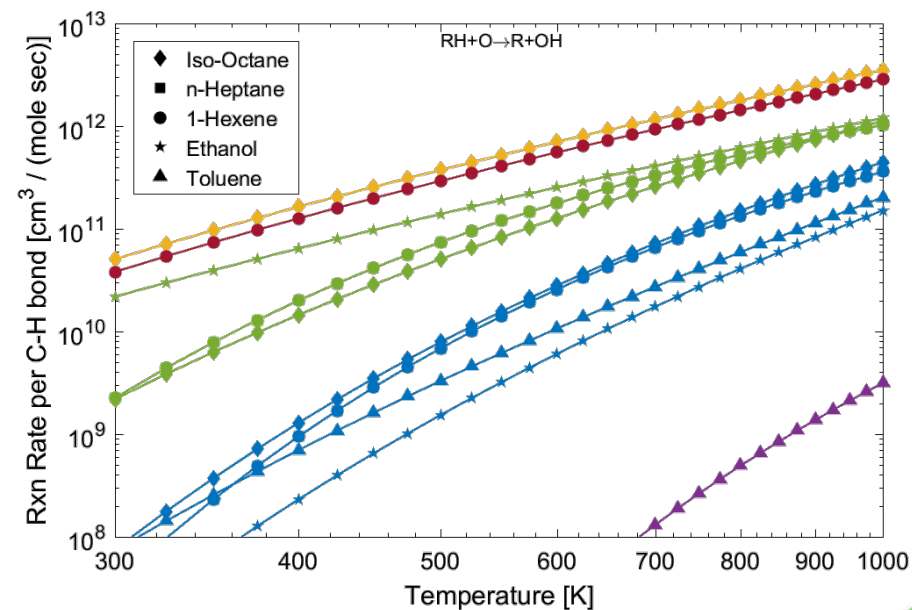
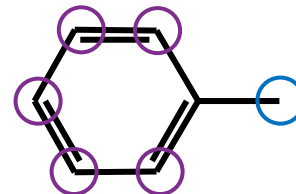
n-Heptane: 15% (17.8 vol%)



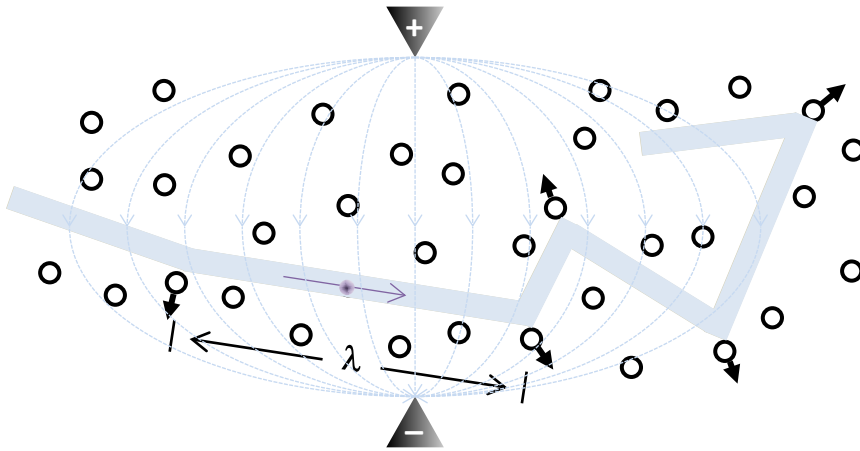
Ethanol: 21% (9.9 vol%)



Toluene: 23% (19.7 vol%)



LTP physics overview



Parameters

Mean free path: $\lambda \propto 1/N \propto T/P$
 Electric field : $|E| \propto \text{electron acceleration}$
 Reduced electric field: $|E|/N \propto \text{electron energy}$

Plasma Classification

Thermal: Elastic energy transfer $\Rightarrow T_e \approx T_{\text{gas}}$
 Non-thermal: Electron energy transfer $\Rightarrow T_e \gg T_{\text{gas}}$

Electron energy transfer mechanisms

Vibrational-to-translational relaxation: **slow**
 Electronic gas heating: **fast**
 Chemical ionization/dissociation: **fast**

Inductive Spark



Image: NGK

RF Corona



Image: BorgWarner

Transient Plasma

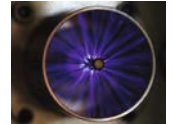
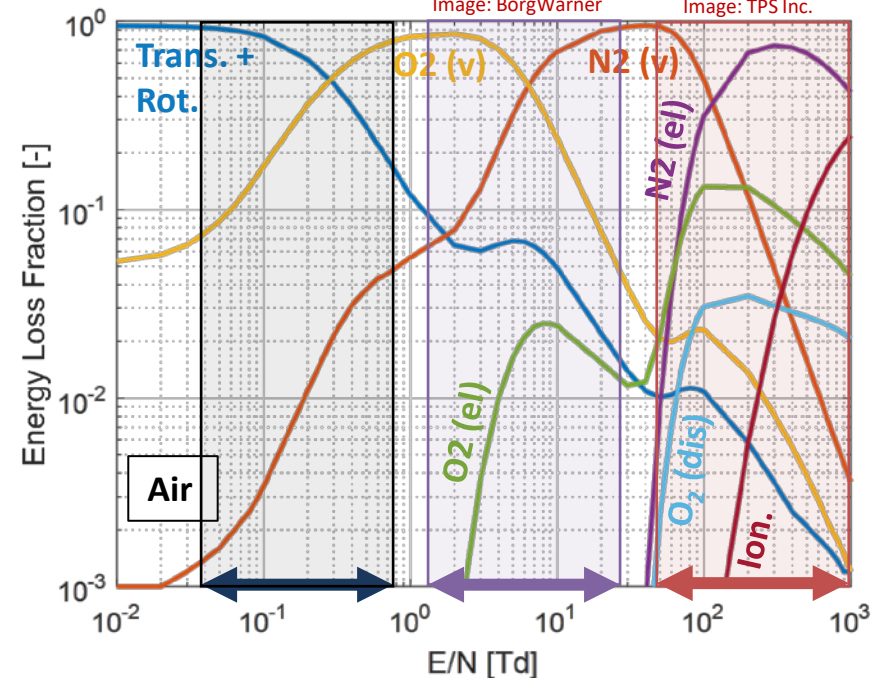


Image: TPS Inc.



Gas Temperature: ~ 10000 K

~ 2500 K

~ 1000 K

Technical Backup Slide: Argonne engine experiments

NGK
Conventional Spark



Current Focus

TPS Inc.
Close-Coupled PND

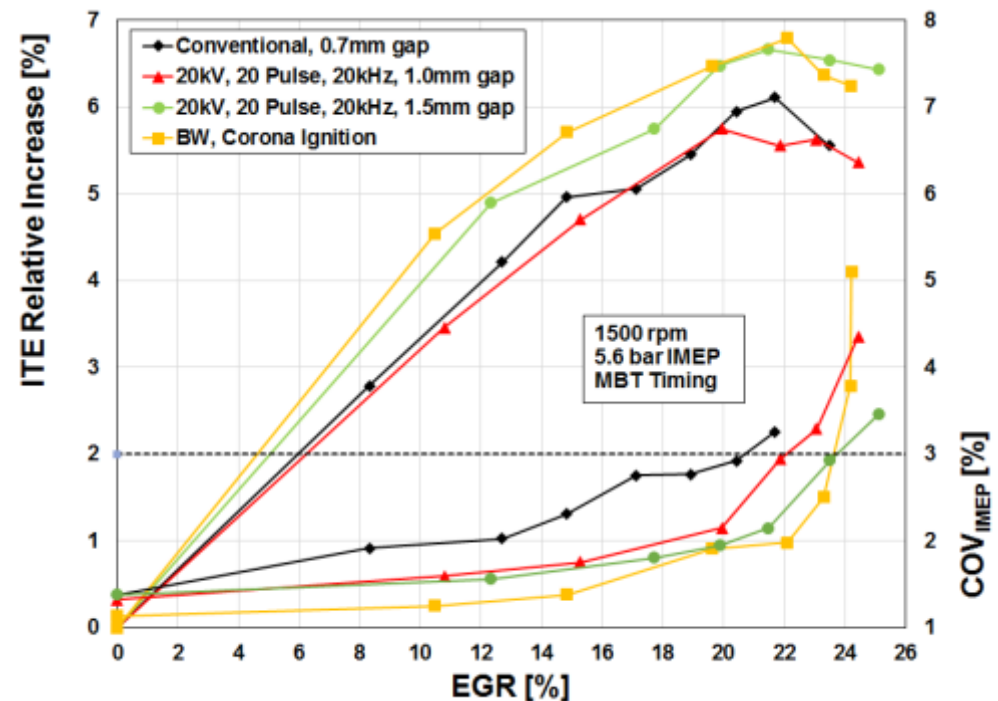


BorgWarner
EcoFlash RF Corona



Displacement	0.6 L
Bore x Stroke [mm]	89.04 x 100.6
Compression Ratio	12.1:1

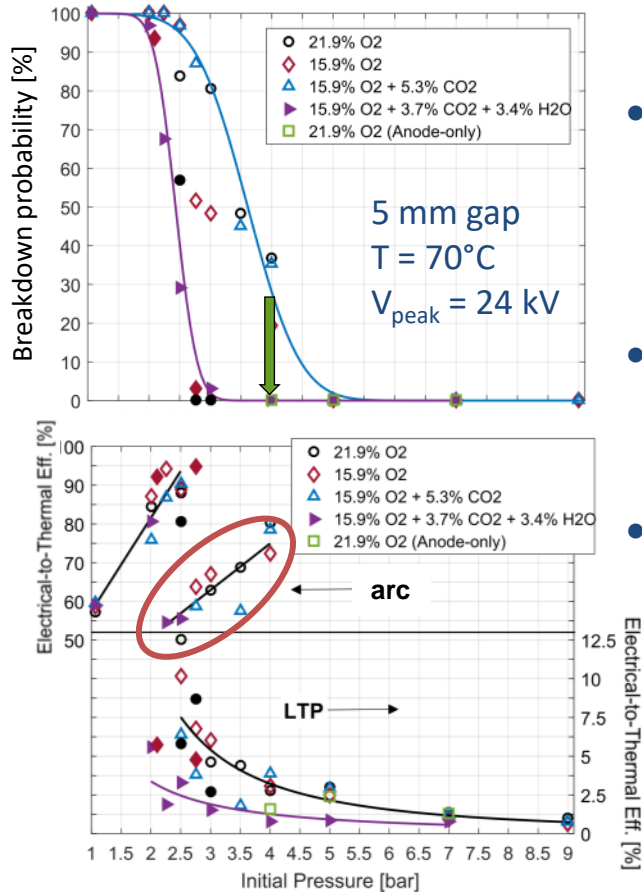
Similar results found
for lean operation



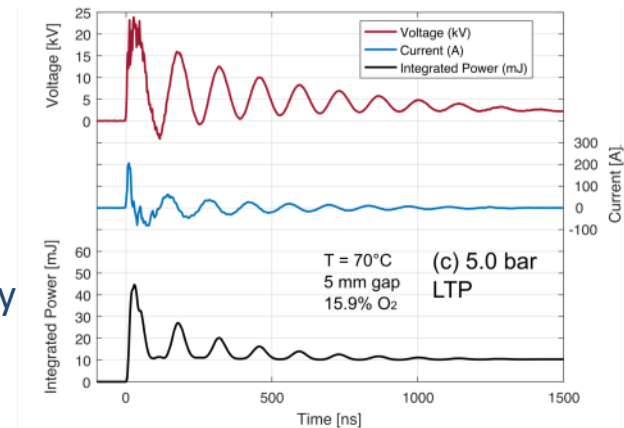
- What is the ignition mechanism?
- How does EGR influence discharge phenomena?
- What prevents further dilution limit extension?

FY17 ACS006: Arc transition

Note: solid symbols from a different ultra air bottle



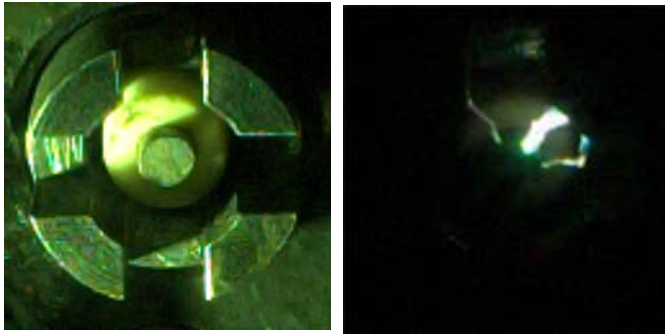
- Minimal impact of gas composition on arc probability
- Anode-only configuration lowers the breakdown limit
 - Apparent arcs along the insulator occur at low densities
- Large reduction in breakdown transition density w/ added H₂O (coincided w/ a changed in ultra-air bottle)
 - Could be lower argon content (no spec. for ultra zero air)
 - We have switched to desiccated house air
- Very efficient electric-to-thermal energy transfer during arc
 - Delayed arc due to pulse voltage/current oscillations
- Lower electric-to-thermal energy transfer for LTP
 - Exponential decay in energy transfer w/ increased density
 - Heating still comparable to inductive coil systems



Basic Tests

FY17 ACS006: Multi-pulse hysteresis for nanosecond TPI

Sjöberg et al, *SAE Int J Engines*, 2014

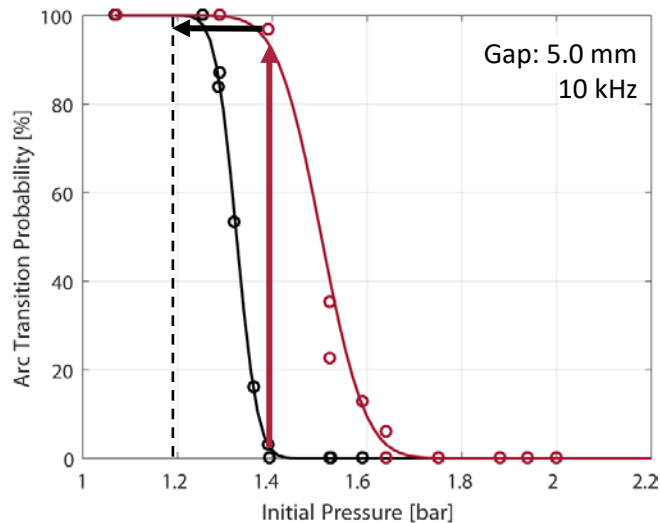


Arcs with multi-pulse – no arc with single-pulse
⇒ a thermal or chemical pre-conditioning mechanism

$$\Delta T = \frac{\overset{\text{Calorimetry}}{E_{\text{Thermal}}}}{\rho c_p V}$$

Minimal heat transfer between pulses

- +15% temp. @ 2nd pulse
- predicted arc probability: 100%

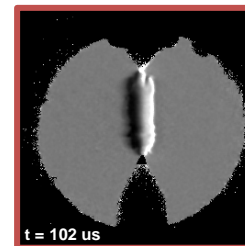


Wolk & Ekoto, *IAV Conference on Ignition Systems*, 2016.

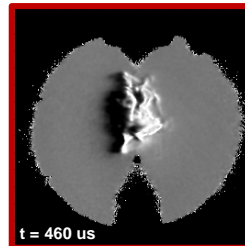
Engine results confirmed by calorimetry



Inductive Spark
Laminar expansion



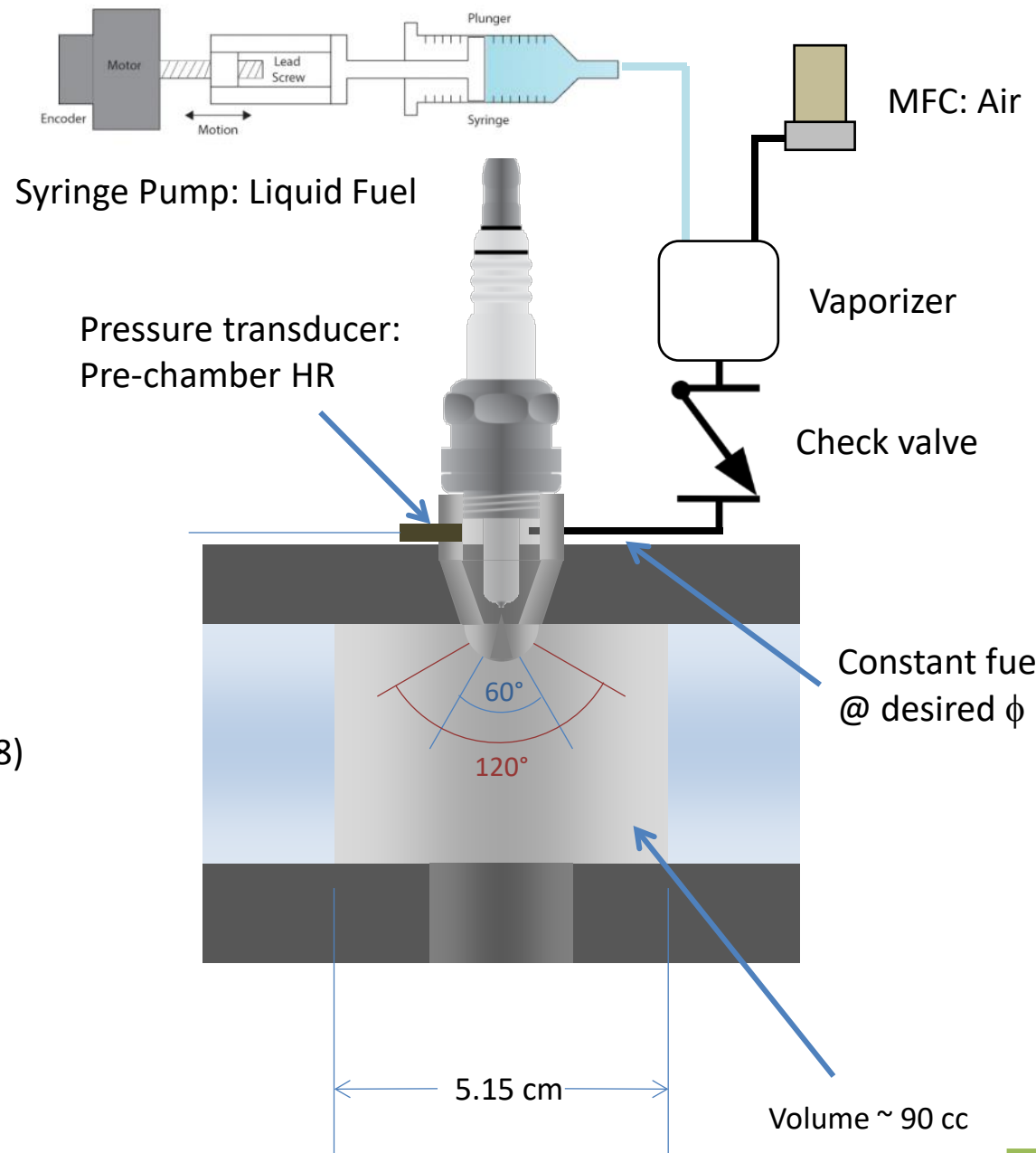
Nanosecond Discharge
Turbulent expansion



Impact: Extended dilution limits with nanosecond discharges attributed to arc-induced faster kernel growth rates – not LTP physics.



TJI Calorimeter



Things to evaluate

- Nozzle angle
 - narrow bowl
 - wide chamber
- Nozzle hole # & area
- Pre-chamber ϕ
- Fuel type
 - gaseous (e.g., CH₄, C₃H₈)
 - Liquid (e.g. IC₈, EtOH)
- What else?
- Pre-chamber volume (2-3 cc)
- Pre-chamber composition
- Combustion
 - Jet strength vs. jet products